

A MODEL FOR CALCITE PRECIPITATION IN AN ELEVATED GEOTHERMAL GRADIENT AT YUCCA MOUNTAIN OVER 10 MILLION YEARS

Eric Sonnenthal and Tianfu Xu

Contact: Eric Sonnenthal, (510) 486-5866, elsonnenthal@lbl.gov

RESEARCH OBJECTIVES

In an earlier study, Xu et al. (2003) simulated the precipitation of calcite in the unsaturated zone (UZ) of Yucca Mountain over a ten million year (Ma) period and compared the results to data collected by the U.S. Geological Survey. The objective of this study was to evaluate the relationship between infiltration rate and calcite abundance; therefore, simulations were performed using the present-day geothermal gradient and a range of infiltration rates. Abundant evidence indicated that the majority of the calcite in the UZ precipitated from downward flowing water of meteoric origin. Recent fluid-inclusion data (from University of Nevada, Las Vegas) showed that calcite precipitated under elevated temperatures for several Ma. Temperatures in the Topopah Spring Tuff at the level of the Exploratory Studies Facility (ESF) prior to approximately 6 Ma may have been around 45–60°C, with a maximum value of 83°C. The latter findings have been used as evidence by some that hydrothermal circulation of upwelling fluids was responsible for the calcite. This new study evaluates the effect of an elevated geothermal gradient on calcite precipitation in the Yucca Mountain UZ.

APPROACH

Based on the temperature history inferred from fluid inclusions, a variable temperature lower boundary at the water table was developed to approximate the inferred paleotemperatures in the Topopah Spring Tuff. The temperature was set initially at 95°C at the base of the 1-D model at 10 Ma and allowed to decrease through conductive and advective cooling into the overlying rock and with the atmosphere. The infiltration rate was set to 5.92 mm/yr with a simplified geochemical system composed of primarily calcite and silica polymorphs as well as several aqueous and gaseous species. The simulation was carried out using the nonisothermal reactive geochemical transport code TOUGHREACT developed at Berkeley Lab.

ACCOMPLISHMENTS

Simulated calcite abundances under elevated temperatures, compared to those for the ambient geothermal gradient and the measured values, are shown in Figure 1. Somewhat greater abundances result from higher temperatures, yet the overall pattern and magnitude is similar to that for the steady-

state ambient temperature distribution. Higher temperatures result in lower calcite solubility and somewhat higher calcite abundances, yet the abundances are dominated by the Ca flux into the unsaturated zone. The variable temperature simulation equally captures the U.S. Geological Survey measured data for the TCw, TSw, and CHn hydrostratigraphic units, and equally overestimates abundances in the PTn. Such deviations in the PTn may result from processes not treated in the simulations, such as reactions with feldspars and glass, and cation exchange with zeolites.

SIGNIFICANCE OF FINDINGS

Even with a temperature of 95°C at the base of the UZ, the system remains unsaturated and gravity-driven flow is dominant, as opposed to hydrothermal circulation in saturated systems driven by differences in fluid density. The elevated temperatures showed somewhat greater abundances of calcite in most units compared to those at ambient temperature, yet the trends with depth are similar and did not change the overall relationship between calcite abundance and infiltration rate (as documented in the first study). Thus, the current study provides support for the widely held view that calcite precipitation was the result of downward infiltrating meteoric water at long-term average rates on the order of 10 mm/yr.

RELATED PUBLICATIONS

Sonnenthal, E., and T. Xu, Reply to "Commentary: Assessment of past infiltration fluxes through Yucca Mountain on the basis of the secondary mineral record—is it a viable methodology?" by Y.V. Dublyansky and S.Z. Smirnov. *Journal of Contaminant Hydrology*, 77, 225–231, 2005. Berkeley Lab Report LBNL-57290.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

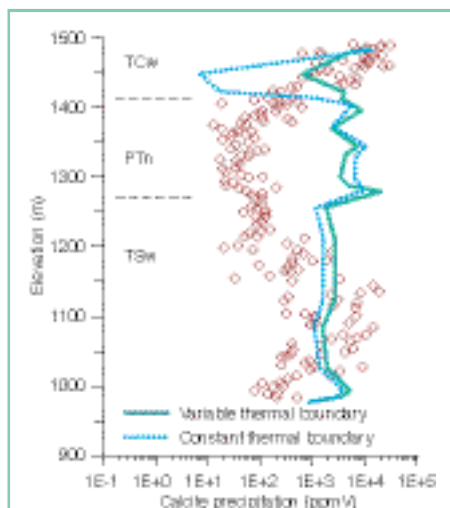


Figure 1. Total (fracture plus matrix) calcite abundances (volume fraction) obtained with two types of thermal conditions applied at the bottom boundary (WT-24 column, after 10 million years). Diamonds represent bulk rock calcite abundances measured by the U.S. Geological Survey.

